Process design optimization strategy to develop energy and cost correlations of CO_2 capture processes

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Abstract

In the context of CO_2 emissions reduction from power plants, CO_2 removal from flue gas by chemical absorption with monoethanolamine is analyzed in detail. By applying process integration and multi-objective optimization techniques the influence of the operating conditions on the thermo-economic performance and on the optimal thermal integration within a power plant is studied. With the aim of performing optimization of complex integrated energy systems, simpler parameterized models of the CO_2 capture process are developed. These models predict the optimized thermo-economic performances with regard to the capture rate, flue gas flowrate and CO_2 concentration. When applied to overall process optimization, the optimization time is considerably reduced without penalizing the overall power plant model quality. This approach is promising for the preliminary design and evaluation of process options including a CO_2 capture unit.

Keywords: CO_2 capture, Chemical absorption, Blackbox model, Multi-objective optimization, Process design

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Nomenclature

Abbreviations

CC Carbon Capture

CCS Carbon Capture and Storage

FGR Flue Gas Recirculation

GT Gas Turbine

LHV Lower Heating Value

MEA Monoethanolamine

NG Natural Gas

NGCC Natural Gas Combined Cycle

Greek letters

Δh^o Lower heating value, kJ/kg

ϵ_{tot} Energy efficiency, %

η_{CO2} CO_2 capture rate, % or -

ξ_{CO2} CO_2 concentration, -

Roman letters

COE Electricity production cost, \$/GJ_e

d Diameter, m

$\dot{E}$ Mechanical/electrical power, kW

I Capital investment cost, \$

$\dot{m}$ Mass flow, kg/s

$\dot{n}$ Molar flow, kmol/s

N Number of stages, -

P Pressure, bar

h	Height, m
$\dot{Q}$	Heat, kW
T	Temperature, K

Subscripts

cc	plant with carbon capture
ref	reference plant without carbon capture

Superscripts

$^{+}$	Material/energy stream entering the system
$^{-}$	Material/energy stream leaving the system

1. Introduction

For reducing CO_2 emissions from power plants, CO_2 capture and storage (CCS) is considered as a promising option. The most common technology to capture CO_2 is chemical absorption with amines, especially monoethanolamine (MEA). This process requires however a significant amount of energy for solvent regeneration which penalizes the efficiency of the electricity production. The impact of CO_2 capture on the process performance can be assessed by thermo-economic analysis, including heat and power integration of the capture process and the related investment estimation. Changing the design conditions of the ab- and desorption columns together with the flow of amines reveals to be sensitive to convergence and heavy in computation time, especially when the optimization is to be done together with the variation of the CO_2 concentration and with the purpose of finding the best economical design from the CO_2 capture point of view. Recent studies have investigated the potential of replacing complex unit models of highly non-linear processes by compact yet accurate surrogate models reproducing the results of the rigorous model in a fraction of the simulation time without losing accuracy [1–4]. In [4] it is shown how reduced order models based flowsheet optimization can increase the efficiency of energy processes.

This paper presents an approach to develop a blackbox model of the CO_2 capture unit predicting the investment, as well as the heat demands and their temperature levels required for the combined heat and power integration model, by using correlations and neural networks that are drawn from the optimization results of the complex first-principle CO_2 capture unit model. The advantage of this approach with regard to the optimization problem formulation is that the optimized CO_2 capture subproblem can be introduced in a larger process to perform optimizations of the global problem, and with regard to energy integration, that information about the heat demand and the temperature levels are conserved. This approach is applied to study a natural gas combined cycle process (NGCC) with flue gas recirculation (FGR) and CO_2 capture (CC).

2. Methodology

The approach to develop a simpler parameterized model of the CO_2 capture unit (i.e. subproblem) to be used in the overall process design optimization (i.e. global problem) is implemented using process design techniques combining process modeling with established flowsheeting tools, and process integration in a multi-objective optimization framework as illustrated in Figure 1. The thermo-economic modeling methodology follows the principles explained in [5, 6]. The main feature of this approach allowing to assemble different process models in a superstructure, is the dissociation of the technology models from the analysis models. The models are organized as an input-output entity and structured data is transferred between the different models. In the energy integration model, the heat recovery in the system and the combined heat and power production is optimized as described in [7]. The economic model includes the equipment sizing and the capital cost estimation based on the correlations given in [8, 9]. To evaluate the environmental impacts, the local CO_2 emissions are considered, knowing that the whole life cycle impacts could be assessed following approach described in [10].

The flowsheet of the CO_2 capture by chemical absorption with monoethanolamine (MEA) is illustrated in Figure 2 and described in more detail in [11]. The amine solvent neutralizes the acidic compounds in the absorber. After being heated up, the saturated solution passes in the stripper where the chemical bounds are broken, the acid gas is released and the solvent is recovered for reuse in the absorber. A considerable amount of energy is consumed for the regeneration of the solvent, the compression of the flue gas and the pumping of the amine. The developed first-principle CO_2 capture model is based on the Aspen-Plus rate-based model adapted from the default model available from AspenTech [12]. CO_2 compression to 110 bar is not included in the capture unit itself, but accounted in a separate model. A CO_2 purity of over 98%wt is targeted from a typical post-combustion flue gas consisting mainly of N_2, CO_2, excess O_2 and water. The CO_2 capture unit performance is expressed by the investment cost I, the CO_2 capture rate ($\eta_{CO2} = \frac{\dot{n}_{CO2captured}}{\dot{n}_{CO2,inFG}}$) and the energy demand (i.e. reboiler duty $\dot{Q}_{LP}$, electricity $\dot{W}$) and is essentially influenced by the design decision variables given in Table 1. The selected input variables for the simpler parameterized blackbox model reflecting the process behavior are the flue gas mass flow ($\dot{m}_{FG}$) and the CO_2 concentration in the flue gas (ξ_{CO2}) as illustrated in Figure 3. The absorber inlet temperature and pressure are kept constant by a blower and heat exchanger. The only decision variable is hence the CO_2 capture rate (η_{CO2}). Consequently, the number of decision variables of the overall process is smaller than the one for the sub-problem since some parameters are internal to the blackbox system. The output parameters of the blackbox model are the investment, mechanical and thermal energy demand and the associated temperature levels.

2.1. Sub-problem optimization

The CO_2 capture sub-problem is first optimized for different flue gas compositions (ξ_{CO2}: 0.065, 0.074, 0.081 and 0.09wt-) and flows ($\dot{m}_{FG}$: 655, 955, 1455, 1955, 2455 and 2955 kg/h). The multi-objective optimization problem is solved by applying an evolutionary algorithm [13] computing a set of optimal solutions in the form of a Pareto front. The objectives are to maximize the CO_2 capture rate η_{CO2} and to minimize the capital investment I with regard to the decision variables in Table 1. It is assumed that the objectives are not influenced by the pressure drop and the heat load. It has been demonstrated by sensitivity analysis that minimum pressure drops and heat loads are correlated with the maximum CO_2 capture rate which justifies this assumption. The Pareto optimal frontiers computed for the different process configurations are illustrated in Figure 4. The influence of the flowrate on the equipment size and consequently on the investment is strongly reflected. Moreover, the investment is slightly affected by the CO_2

capture rate. Based on these optimization results of the first-principle MEA unit model, the goal is to develop a simplified parameterized blackbox model (Figure 3) predicting the process performance accurately.

2.2. Surrogate model development

By fitting the generated Pareto fronts (Figure 4), regression correlations and neural networks are defined to predict the thermo-economic performances of the CO_2 capture unit with regard to the input variables η_{CO2} (x_1), $\dot{m}_{FG}$ (x_2) and ξ_{CO2} (x_3). Statistical tests are carried out to validate the proposed correlations. The F statistic is applied to test the model validity against the assumption that at least one coefficient of the correlation is significant. In addition, the validity of each coefficient is verified by the *t*-test following a Student's t distribution, if the null hypothesis is supported. The approach is illustrated here for setting up the investment cost correlations. The development of the correlations for the mechanical power, the heat load and the temperature levels follows the same approach.

2.2.1. CO_2 capture investment cost correlation

The goal is to develop a correlation of the investment I with regard to the input variables: I=$f(\eta_{CO2},\dot{m}_{FG},\xi_{CO2})=f(x_1,x_2,x_3)$. It is to note that the developed correlations for the investment cost do not follow the conventional cost estimation approach since they deal with the optimized investment computed from simulation with regard to certain decision variables. Three different approaches for fitting are compared.

Polynomial fit. In a first attempt, multi-dimensional polynomial correlations are set up. Therefore, correlations are drawn for each data series with fixed

ξ_{CO2} (I=$f_{\xi_{CO2}}(\eta_{CO2},\dot{m}_{FG})$) based on Eq.1 yielding coefficients of determination R^2 values around 0.98. According to the statistical tests, additional terms do not improve the goodness of fit. To include the variation with regard to ξ_{CO2} a linear variation of the coefficients p_i in Eq.1 ($p_i = \kappa_{i,1} + \kappa_{i,2}\xi_{CO2}$) is first assumed. The statistical tests results reported in Table 2 show that some terms are not significant which leads to the final expression given by Eq.2.

$$f_{x3}(x_1, x_2) = p_{00} + p_{10}x_1 + p_{01}x_2 + p_{20}x_1^2 + p_{11}x_1x_2 \quad (1)$$

$$f(x_1, x_2, x_3) = k_0 + k_1x_1 + k_2x_2 + k_3x_1x_2 + k_4x_1x_3 + k_5x_2x_3 + k_6x_1x_2x_3 + k_7x_1^2x_3 \quad (2)$$

Sortcut fit. In a second attempt, a correlation based on a shortcut model including the known physical relations in the absorption and desorption columns is set up. The number of stages is related to the absorbed fraction through the Kremser equation (Eq.3) assuming stage equilibrium instead of rate-based model, which allows together with the flue gas mass flowrate $\dot{m}_{FG}$ to estimate the diameter d and height h through column design heuristics and consequently the investment costs I (Eqs 4-6). The constant parameters in these functions are defined by solving a minimization problem in the least-square sense. A hybrid method combining mathematical programming and evolutionary algorithm for finding a good initial point has been used for this purpose.

$$N = a_1 log\left(\frac{a_2}{1-\eta_{CO2}} + a_3\right) + a_4 \quad (3)$$

$$d = f(\dot{m}_{FG}, \xi_{CO2}) \tag{4}$$

$$h = f(N, d) \tag{5}$$

$$I = f(h, d) \tag{6}$$

Neural network. As a last approach, the neural network (NN) fitting tool from matlab using the Levenberg-Marquardt backpropagation algorithm for network training has been applied on the optimization results dataset (i.e. training 55% of data, validation 25%, testing 20%). The two-layer feed-forward network with sigmoid hidden neurons and linear output neurons illustrated in Figure 5 reveals to be well suited to fit such multi-dimensional mapping problems.

Fit results. The goodness of fit of these approaches is compared in Figure 6 for the capital investment. The different fits give a good estimation of the investment costs since the results are closely distributed around the bisectrix of the optimization results.

3. Application: NGCC with CO_2 capture

To illustrate the approach, the integration of post-combustion CO_2 capture in power plants is studied. Therefore, the developed parametrized CO_2 capture blackbox models are integrated with a natural gas power plant (NGCC) model to optimize the process design with CO_2 capture (Figure 1). The investigated process consists of a natural gas reheat gas turbine combined cycle with flue gas recirculation (FGR) and CO_2 capture. To address the flame stability concerns at high FGR, pure hydrogen or syngas can be injected. The H_2 production is modeled by a high temperature oxygen separation membrane autothermal reforming reactor.

3.1. Performance indicators

The performance of the overall process comprising the integration of the parameterized CO_2 capture models, is compared based on thermo-economic considerations assessing also the energy and economic costs of capturing CO_2 and the impact of CO_2 recirculation. The energy efficiency ϵ_{tot} is defined by the ratio between the net electricity output and the resources energy input according to Eq.7. The electricity production costs include the annual capital investment and the operation and maintenance costs calculated with the assumptions given in Table 3. The CO_2 mitigation potential is assessed by the overall CO_2 capture rate η_{CO2} and the CO_2 avoidance cost. The overall CO_2 capture rate is lower than the internal CO_2 capture rate of the chemical absorption since some CO_2 is emitted during the H_2 production. The CO_2 avoidance costs expressed by Eq. 8 are defined by the difference of the CO_2 emissions and the difference of the total costs with regard to the reference power plant without CO_2 capture (noCC).

$$\epsilon_{tot} = \frac{\Delta E^-}{\Delta h^0_{NG,in} \cdot \dot{m}_{NG,in}} \tag{7}$$

$$\$/t_{CO2,avoided} = \frac{COE_{CC} - COE_{noCC}}{CO_{2,emit_{noCC}} - CO_{2,emit_{CC}}} \frac{[\$/GJ_e]}{[t_{CO2}/GJ_e]} \tag{8}$$

3.2. Base case comparison

The performance of the post-combustion CO_2 capture in the NGCC power plant is first assessed with the first-principle MEA model and then compared with the results obtained with the different blackbox models. For these base case configurations around 50% of FGR and around 85% CO_2 capture are considered. Sensitivity analyses have revealed that FGR does not considerably impact the process efficiency but improves the economics of CO_2 capture by increasing the CO_2 concentration in the flue gas and reducing therefore the CO_2 capture costs. The performance results are summarized in Table 4 and compared to the corresponding conventional NGCC plant without CO_2 capture. It is shown that CO_2 capture decreases the efficiency by over 8% points and increases the production costs by up to one third. These results are in the same range as the one given in [14] reporting for a conventional NGCC an efficiency of 56.6%, CO_2 emissions of $102.8\mathrm{kg}_{CO2}/\mathrm{GJ}_e$ and COE of $21.3\$/\mathrm{GJ}_e$ and for a NGCC with post-combustion CO_2 capture an efficiency of 48.4%, CO_2 emissions of $15.3\mathrm{kg}_{CO2}/\mathrm{GJ}_e$ and COE of $28.3\$/\mathrm{GJ}_e$.

The results obtained with the blackbox models are comparable to the one obtained with the first principle model. The shortcut fit yields the best estimation of the production costs. The deviation of around 2.7% is negligeable compared to the error range of the equipment costs estimations. With the neural network model, the assessed efficiency is about 3.5% lower than the efficiency computed by the first principle model. While, for the other parameterized models the deviation is less than 2.5%. This variation is due to the differences in the heat load estimations illustrated by the composite curves comparison in Figure 7. The neural network model slightly overestimates the reboiler heat duty which results in a lower efficiency. These simplified parametrized blackbox models allow to evaluate the penalty of CO_2 capture on the power plant performance quite accurately. The major advantage of using these simplified models is the significant reduction of the computation time as shown in Table 5. Once the blackbox models are set up, the computation time is reduced by over 45% for one computation. Consequently, these simplified models allow to make a preliminary analysis of CO_2 capture process options.

3.3. Global problem optimization

To study the influence of CO_2 capture and flue gas recirculation on the power plant performance in more detail, a multi-objective optimization of the global problem is performed. The objectives are the minimization of the electricity production costs (COE) and the maximization of the overall CO_2 capture rate (η_{CO2}). The decision variables for the power plant are the flue gas recirculation and in case where syngas has to be injected the hydrogen production temperature and the steam to carbon ratio. Since the flue gas flowrate and the CO_2 concentration are defined by the power plant model, the number of decision variables for the parameterized CO_2 capture model is reduced to one, the CO_2 capture rate, compared to 15 for first principle MEA model (Table 1). By using the blackbox models calibrated on the subproblem optimization results for the optimization of the global system, the hypothesis is made that for a given CO_2 capture rate the optimal solution corresponds to the minimal investment. The generated Pareto fronts in Figure 8 reveal the trade-off between the CO_2 capture rate and the electricity production costs. This trade-off is explained by the reduced electricity output due to the energy demand for solvent regeneration and CO_2 compression yielding a lower efficiency, and the increased capital investment costs for the capture equipment.

Compared to the optimization problem results including the first-principle MEA unit model (MEA model), the accuracy is nearly maintained for the problems including the different balckbox models up to 87% of CO_2 capture as illustrated by Figure 8. The comparison of the results in Table 6 for compromise Pareto solutions yielding a CO_2 capture rate of 87%, shows that the generated process configurations are similar. In fact, the optimized values of the FGR differ by less than 2%. For a chosen process configuration, the detailed CO_2 capture unit design can be recomputed subsequently based on the first principle CO_2 capture model. The values of the required input parameters defined in Table 1 can be approximated from the data series used for the blackbox models calibration (section 2.1) based on a griddata approach. The overall performance, design and operating conditions assessed in this way for the compromise configurations obtained through optimization of the power plant with the parameterized CO_2 capture models are very close to the one resulting from the optimization with the first principle CO_2 capture model. This high concordance is shown by the composite curves in Figure 9. This reveals that the sub-problem optimum is included in the global problem optimum for solutions having a CO_2 capture rate below 87%.

At high CO_2 capture rates, there is however a divergence in the solutions. The optimization of the power plant performance with the parameterized CO_2 capture models leads to process designs with low FGR (<12%), while the optimization with the first-principle CO_2 capture model favors FGR above 50% at high CO_2 capture rates. This difference in the design of the power plant leads to a different design of the CO_2 capture unit due to the changes in the CO_2 concentration and the flue gas flow rate. Consequently, the assessed efficiencies and costs diverge. When recomputing the solution generated by the parameterized blackbox model with the first principle MEA model, a process design with a lower CO_2 capture rate (83% instead of 90%), higher efficiency and lower productions costs is obtained. This indicates that the hypothesis that the sub-problem optimum is included in the global problem optimum is not valid for high CO_2 capture rates. In fact, there is a compromise between the investment and the energy demands, which both affect the production costs. Consequently, it is possible to find for a given CO_2 capture rate a solution with a higher capital investissment yielding a higher efficiency and lower COE. By recalcuating the optimal solution found with the first-principle model with the parameterized model, the solution yields a higher specific production cost per ton of CO_2 captured than the optimal solution found with the parameterized model. This explains why this solution has not been retained during the optimization with the parameterized model. In fact the parameterized model can not find this solution. In order to reflect this bahaviour in the parameterized blackbox models, a solution would be to calibrate these models on the minimzation of the production costs accounting the heat demand at its exergy value, or on the minimization of the exergy losses instead of the investment. Once the Pareto sets are generated with the modified objective function, the blackbox models of the CO_2 capture unit can be set up following the approach described previousely. The hypothesis of the optimality of the subproblem in the global problem has hence to be valid in order to take advantage from the reduction of the number of decision variables of the parameterized model in the global problem optimization.

Using the simple blackbox models in the global problem optimization, has the advantage of reducing the computation time considerably. If the same number of evaluations is considered for each optimization problem the computation time is reduced over 45% (Table 5). However, because of the changes in the number of decision variables, the number of evaluations for reaching a same level of convergence is different. It is noted that for the optimization of the power plant with the first principle MEA model the convergence of the Pareto front is not considerably improved between 400 and 2000 evaluations. While for the optimization of the power plant with the parameterized CO_2 capture model convergence is nearly reached around 180 evaluations for a same initial population. By taking into account the reduction of the number of evaluations in the optimization, the use of the parameterized model leads to an additional computation time decrease which favors the use of this kind of simplified models in optimization problems formulations. Consequently, such a quick first optimization is appropriate for the preliminary design and evaluation of process options with CO_2 capture.

4. Conclusion

A strategy applying multi-objective optimization for developing energy and cost correlations of CO_2 capture process units is presented. The advantage of this approach is that the simple parameterized models are developed based on optimization results by applying polynomial fitting and neural networks. Consequently, the number of decision variables of the global problem are reduced compared to the sub-problem optimization. Using the parameterized blackbox models of the chemical absorption unit in the global optimization of a power plant with CO_2 capture reduces the complexity and computation time without loosing much accuracy for capture rates up to 87%. The inclusion of predictions of each heat load and the corresponding temperature level is advantageous with regard to the overall process integration. It is shown that the accuracy of the parameterized models highly depends on the model callibration. In fact, the hypothesis that the optimal solution of the global problem corresponds to the minimum investment for a given CO_2 capture rate reveals to be not valid at high capture rates because there is a compromise between capital investment and energy efficiency. A solution would be to calibrate the parameterized CO_2 capture models on the minimization of the production costs accounting the heat demand at its exergy value instead of on the investment. The proposed approach to develop simplified models based on optimization results is promising for the preliminary design and evaluation of process options with CO_2 capture, especially with regard to the computation time reduction and the reduction of the number of decision variables. However, in order to predict the process behaviour accurately in the whole space of the decision variables, the calibration data set has to be chosen in such a way that the hypothesis of the sub-problem optimality is satisfied.

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Table 1: Decision variables and feasible range for optimization.

Operating parameter	Range	Operating parameter	Range
Lean solvent CO_2 loading [kmol/kmol]	[0.18-0.25]	Split fraction [-]	[0-0.7]
Rich solvent CO_2 loading [kmol/kmol]	[0.4-0.5]	Nb stages absorber	[10-17]
Rich solvent pre-heat T [^oC]	[95-105]	Nb stages HP stripper	[8-15]
Rich solvent re-heat T [^oC]	[115-125]	Nb stages LP stripper	[6-10]
LP stripper pressure [bar]	[1.7-2.1]	Absorber diameter [m]	[6-12]
HP / LP pressure ratio [-]	[1-1.5]	HP stripper diameter [m]	[3-6]
MEA % in solvent [-]	[0.3-0.35]	LP stripper diameter [m]	[2-5]
Absorber steam out [kg_{H2O}/t_{FG}]	[306-309.5]		

Table 2: Regression results for the investment cost correlation leading to Eq.2. ($t_{0.95}$[1538]=1.96, $F_{0.95}$[7;1538]=3.23)

	cst	x_1	x_2	$\mathbf{x}_3$	x_1x_2	x_1x_3	x_2x_3	$x_1x_2x_3$	$\mathbf{x}_1^2$	$x_1^2x_3$	R^2	F-value
Coefficient	33.663	-117.33	-1.93E-5	**0**	1.2E-4	-366.04	4.7E-4	-4.5E-4	**0**	796.38	0.977	9565
t-value	-	-12.18	-3.38	**1.64**	14.4	-2.87	7.53	-4.7	**0.45**	6.2		

Table 3: Economic assumptions.

Parameter	Value
Marshall and Swift index	1473
Expected lifetime	25 years
Interest rate	6%
Yearly operation	7500h/year
Maintenance	5% Invest.
Natural gas price	9.7 $/GJ_{NG}$

Table 4: Performance results for different base case scenarios.

Scenario	η_{CO2} [%]	ϵ_{tot} [%]	CO_2 emit [kg/GJ_e]	COE [$\$/GJ_e$]	Avoid. cost [$\$/t_{CO2,avoided}$]
NGCC	0	58.75	105.08	18.32	-
MEA model	85.11	50.3	12.92	22.92	49.89
Polyfit	85.06	49.13	15.72	23.72	60.46
Shortcut fit	85.06	49.13	15.72	23.56	58.62
NN	85.06	48.50	15.92	24.01	63.62

Table 5: Computation time comparison for multi-objective optimization with 400 evaluations and initial population of 30.

Scenario	time 1 run [h:mm:ss]	time moo [h:mm:ss]
MEA model	0:01:57	10:08:33
BB f2	0:01:05	4:54:32
BB fK	0:01:03	4:56:17
BB NN	0:01:04	4:59:11

Table 6: Performance results for compromise solutions.

Scenario	η_{CO2} [%]	ϵ_{tot} [%]	CO_2 emit [kg/GJ$_e$]	COE [\$/GJ$_e$]	Avoid. cost [\$/t$_{CO2,avoided}$]	FGR [-]
NGCC	0	58.75	105.08	18.32	-	0
MEA model	86.94	50.28	16.16	22.80	50.35	0.539
Polyfit	87.02	50.29	12.93	23.20	52.93	0.528
Shortcut fit	87.16	50.6	13.23	22.90	49.90	0.543
NN	87.45	49.90	13.44	23.30	54.40	0.522

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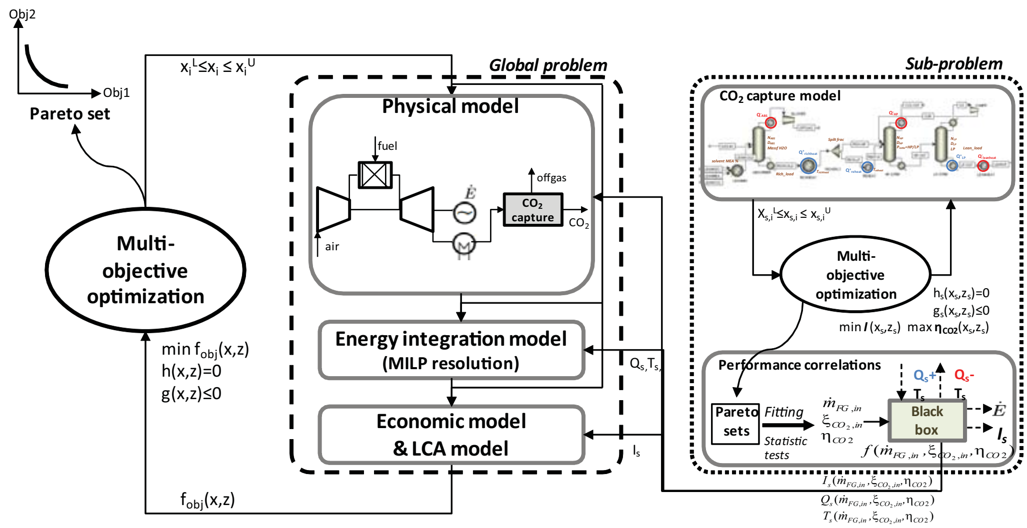

Figure 1: Illustration of the process optimization strategy.

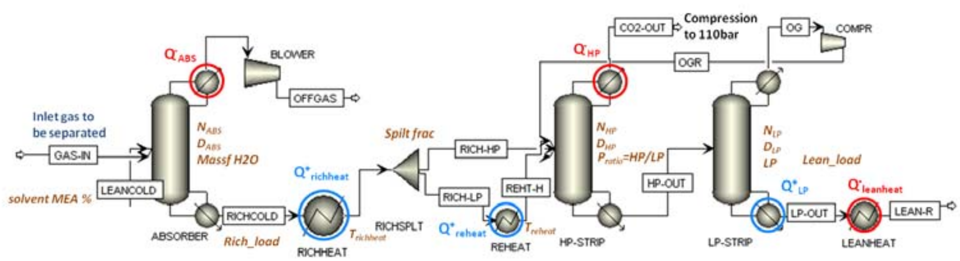

Figure 2: Flowsheet of the CO_2 capture unit implemented in Aspen Plus.

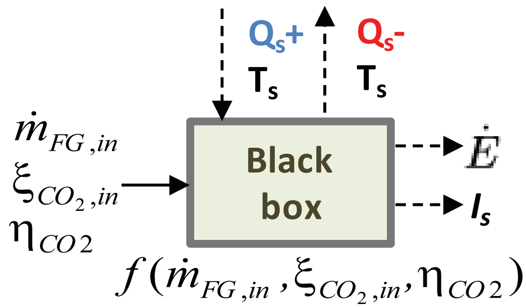

Figure 3: Blackbox model of the CO_2 capture process.

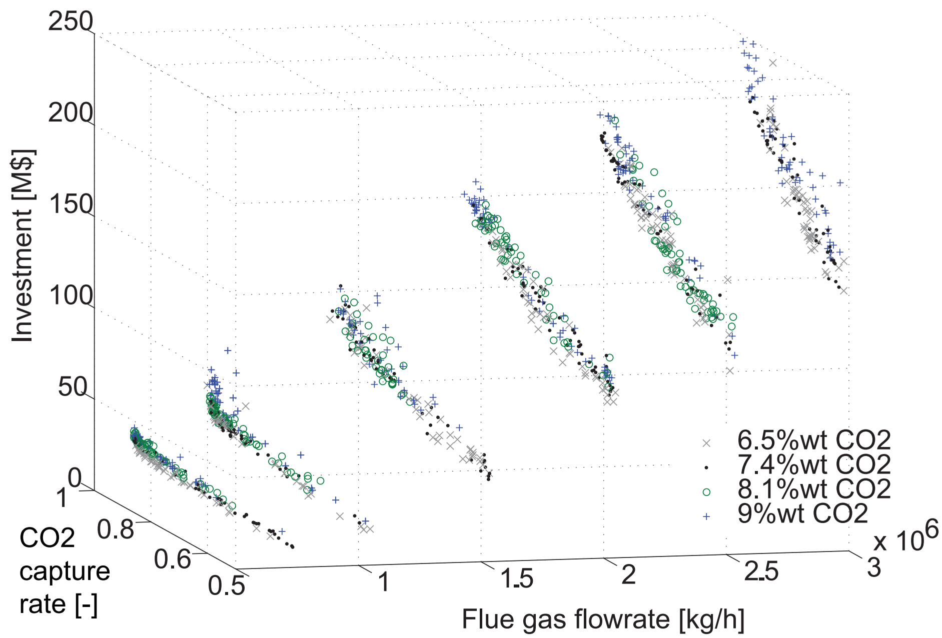

Figure 4: Pareto frontiers showing the trade-offs between investment and CO_2 capture rate for different $\dot{m}_{FG}$ and ξ_{CO2}.

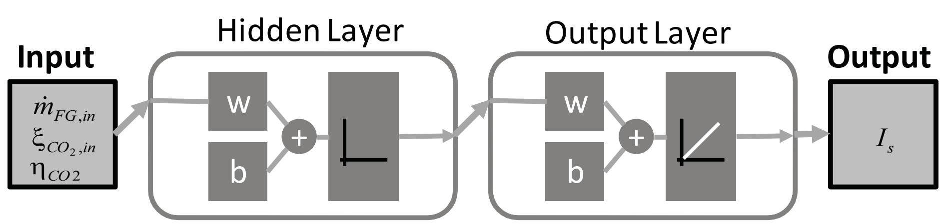

Figure 5: Schematic illustration of neural network.

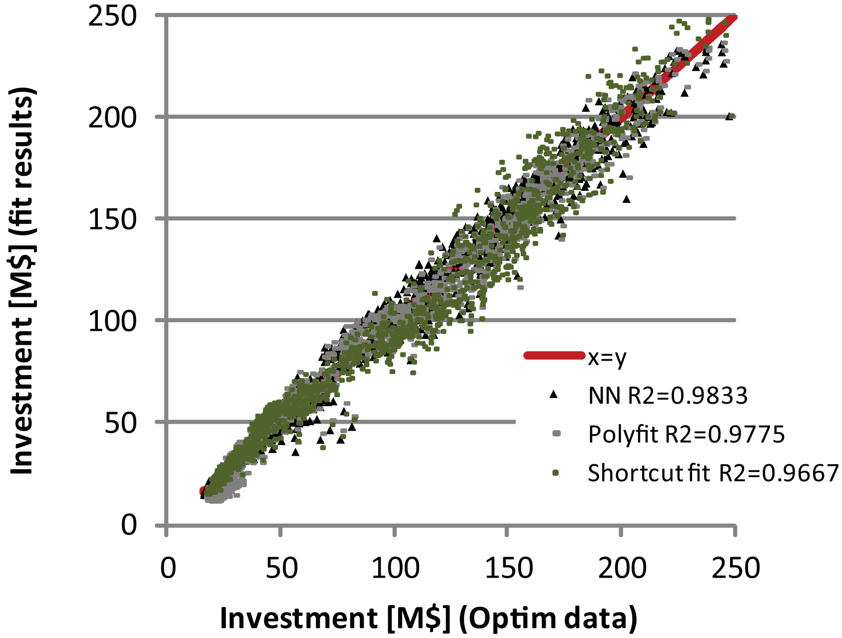

Figure 6: Fitted investment (Polynomial fit - polyfit Eq.2, fit based on shortcut model - shortcut fit, neural network - NN) versus optimization result.

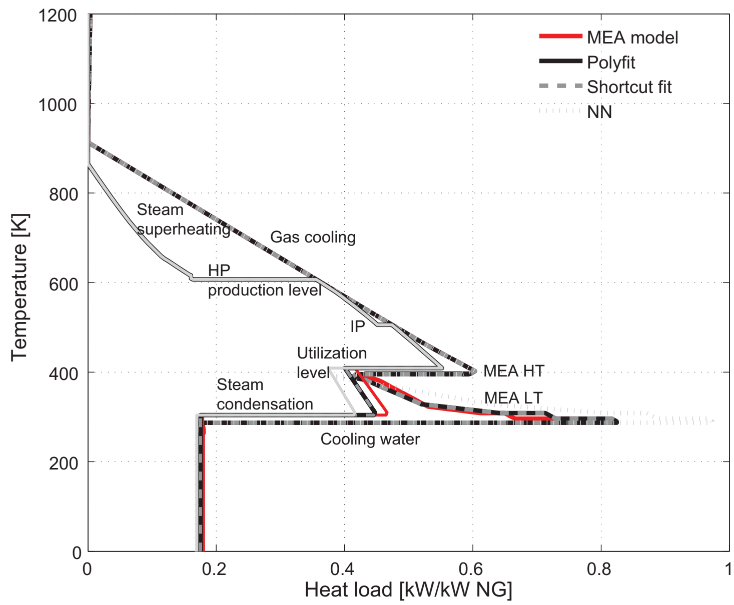

Figure 7: Comparison of composite curves with steam network integration for base case scenarios.

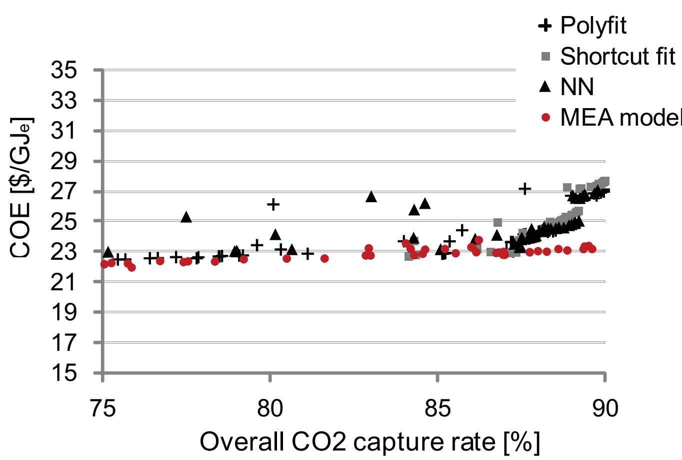

Figure 8: Pareto frontiers of the global problem optimization.

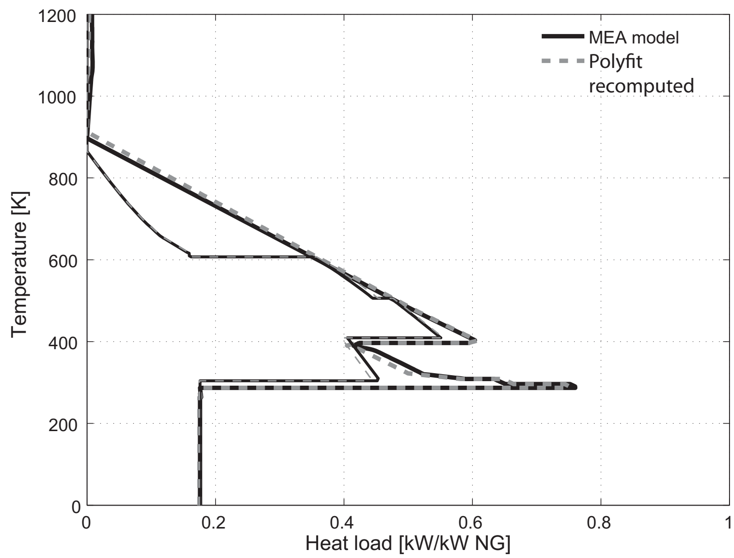

Figure 9: Composite curves for compromise scenario generated by the first principle MEA model through optimization and through recomputation of the parameterized polynomial model with the detailed MEA model.